

Simulation of heavy ion collision using a time-dependent density functional theory including nuclear superfluidity

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Abstract. We carried out a simulation of heavy ion collision using a time-dependent density functional theory. We call it the canonical-basis time-dependent Hartree-Fock-Bogoliubov theory (Cb-TDHFB) which can describe nuclear dynamics in three-dimensional coordinate space, treating nuclear pairing correlation. We simulate $^{20}\text{O}+^{20}\text{O}$ collision using the Cb-TDHFB with a contact-type pairing functional, and show the behavior of gap energy which is decreasing and vibrating while colliding.

1. Introduction

Atomic nucleus is a self-binding finite quantum many-body system whose size is several femtometers ($= \text{fm} = 10^{-15}\text{m}$). It is composed of two kinds of fermions (protons and neutrons) with spin $1/2$ that are called “nucleons”. The number of nucleons in a nucleus is a few hundreds at most. There are about 3,000 nuclei observed in experiments, and yet more to be discovered. In order to study the structure of nuclei, we investigate many excited modes of many nuclei. To study nuclear collision microscopically is also very important. Nucleus has “magic numbers”, which are analogous to those in atoms. This suggests that the nucleon in the nucleus is freely moving in an attractive average potential. The nucleons create the mean field by themselves.

In the time-dependent mean-field theory, the heavy-ion collision is expressed as colliding of two mean fields. We should investigate the behavior of single-particle states while colliding two fields, to expect the structure of nuclei after the heavy-ion collision. Nuclear pairing correlation has a significant role to define single-particle states. It allows the fractional occupation probability of single-particle states due to the pair scattering, which is important to reconstruct a new mean field. The time-dependent Hartree-Fock theory (TDHF) is well-known as a useful tool to study nuclear dynamics[1], however it can not include effects of pairing correlation.

There is a theory to treat pairing correlation in nuclear dynamics self-consistently, which is called the time-dependent Hartree-Fock-Bogoliubov theory (TDHFB). But, there is no study of heavy ion collision using TDHFB with a modern effective interaction in three-dimensional space, because the study is hard to prepare converged initial state, and it needs the huge computational resource[2]. We proposed a new TD mean-field theory to study nuclear dynamics treating pairing, which is named the canonical-basis TDHFB (Cb-TDHFB)[3]. The Cb-TDHFB is derived from full TDHFB equations represented in canonical basis which diagonalizes density

matrix, with Bardeen-Cooper-Schrieffer (BCS)-like approximation for pairing functional (pp, hh -channel). We confirmed that linear response calculations of the Cb-TDHFB are a good approximation of the quasi-particle random phase approximation (QRPA) which is a small amplitude limit of TDHFB[3].

In the present work, we apply the Cb-TDHFB to heavy ion collision in the three-dimensional Cartesian coordinate space using a modern effective interaction (Skyrme: SkM*) with a contact pairing. In the followings, we introduce the Cb-TDHFB equations and the contact pairing functional. Then, we show results of $^{20}\text{O}+^{20}\text{O}$ which indicate an collision of the gap-energy.

2. Formulation and Procedure

2.1. Basic equations and contact pairing

The Cb-TDHFB equations can be derived from the TDHFB equations represented in canonical basis with a simple approximation for pairing functional[3]. The TDHFB equations can be written in terms of the generalized density matrix $\mathcal{R}(t)$ and the generalized Hamiltonian $\mathcal{H}(t)$ [4]. $\mathcal{R}(t)$ composes the one-body density matrix $\rho_{\mu\nu}(t) \equiv \langle \Psi(t) | \hat{c}_\nu^\dagger \hat{c}_\mu | \Psi(t) \rangle$ and the pairing-tensor $\kappa_{\mu\nu}(t) \equiv \langle \Psi(t) | \hat{c}_\nu \hat{c}_\mu | \Psi(t) \rangle$: μ, ν mean arbitrary basis. $\mathcal{H}(t)$ has $h(t)$ and $\Delta(t)$ corresponding to single-particle Hamiltonian and pair potential, respectively. We can express TDHFB state at any time in the canonical (BCS) form as

$$|\Phi(t)\rangle \equiv \prod_{l>0} (u_l(t) + v_l(t) \hat{c}_l^\dagger(t) \hat{c}_{\bar{l}}^\dagger(t)) |0\rangle, \quad (1)$$

where $u_l(t), v_l(t)$ are time-dependent BCS factors and \hat{c}_l^\dagger is a creation operator of canonical basis which diagonalizes density matrix $\rho(t)$. Then, we choose the BCS form of pair potential as

$$\Delta_l(t) = - \sum_{k>0} \kappa_k(t) \bar{\mathcal{V}}_{l\bar{l}, k\bar{k}}, \quad (2)$$

where $\kappa_k(t) \equiv u_k(t)v_k(t)$ corresponds to the pair tensor $\kappa(t)$ in the canonical-basis and $\bar{\mathcal{V}}_{l\bar{l}, k\bar{k}}$ is the anti-symmetric two-body matrix element. The subscripts \bar{l} and \bar{k} mean the pair of canonical basis l and k , respectively. We can obtain the Cb-TDHFB equations from the canonical form Eq.(1) of TDHFB, and with the pair potential Eq.(2), as follows.

$$\begin{aligned} i\hbar \frac{\partial \phi_l(t)}{\partial t} &= (\hat{h}(t) - \eta_l(t)) \phi_l(t), & i\hbar \frac{\partial \phi_{\bar{l}}(t)}{\partial t} &= (\hat{h}(t) - \eta_{\bar{l}}(t)) \phi_{\bar{l}}(t), \\ i\hbar \frac{\partial \rho_l(t)}{\partial t} &= \kappa_l(t) \Delta_l^*(t) - \kappa_l^*(t) \Delta_l(t), \\ i\hbar \frac{\partial \kappa_l(t)}{\partial t} &= (\eta_l(t) + \eta_{\bar{l}}(t)) \kappa_l(t) + \Delta_l(t) (2\rho_l(t) - 1), \end{aligned} \quad (3)$$

where $\eta_l(t) \equiv \langle \phi_l(t) | \hat{h}(t) | \phi_l(t) \rangle + i\hbar \langle \frac{\partial \phi_l}{\partial t} | \phi_l(t) \rangle$. The Cb-TDHFB equations compose the time-evolutions of the canonical basis $\phi_l(t), \phi_{\bar{l}}(t)$, the occupation probability $\rho_l(t) \equiv |v_l(t)|^2$ and the pair probability $\kappa_l(t)$. They conserve orthonormal property of the canonical basis and average particle number. When we choose a special gauge condition $\eta_l(t) = \varepsilon_l(t) = \langle \phi_l(t) | \hat{h}(t) | \phi_l(t) \rangle$, they conserve average total energy.

We introduce neutron-neutron and proton-proton BCS pairing. The BCS pairing matrix elements $\mathcal{V}_{l\bar{l}, k\bar{k}}^\tau$ is written as

$$\begin{aligned} \mathcal{V}_{l\bar{l}, k\bar{k}}^\tau &= \int d\mathbf{r}_1 d\mathbf{r}_2 \sum_{\sigma_1, \sigma_2} \phi_l^*(\mathbf{r}_1, \sigma_1) \phi_{\bar{l}}^*(\mathbf{r}_2, \sigma_2) \hat{\mathcal{V}}^\tau(\mathbf{r}_1, \sigma_1; \mathbf{r}_2, \sigma_2) \\ &\quad \times [\phi_k(\mathbf{r}_1, \sigma_1) \phi_{\bar{k}}(\mathbf{r}_2, \sigma_2) - \phi_{\bar{k}}(\mathbf{r}_1, \sigma_1) \phi_k(\mathbf{r}_2, \sigma_2)]. \end{aligned} \quad (4)$$

We introduce the spin-singlet contact interaction to Eq.(4):

$$\hat{V}^\tau(\mathbf{r}_1, \sigma_1; \mathbf{r}_2, \sigma_2) \equiv V_0^\tau \frac{1 - \hat{\boldsymbol{\sigma}}_1 \cdot \hat{\boldsymbol{\sigma}}_2}{4} \delta(\mathbf{r}_1 - \mathbf{r}_2), \quad (5)$$

where τ indicates neutron or proton channel and V_0^τ is a strength of pairing[5]. In this present work, we do not use the time-reversal relation between l - and \bar{l} -canonical basis.

2.2. Procedure and calculation space

At first, we prepare the initial states (HF or HF+BCS ground states) with the wave functions for projectile and target at some impact parameter b at distance where they feel only Coulomb interaction. Then, we boost the wave functions and translational calculate the time-evolution of nuclear densities to obey Eq.(3). In this present work, we use the three-dimensional Cartesian coordinate-space representation for the canonical states, $\phi_l(\mathbf{r}, \sigma; t) = \langle \mathbf{r}, \sigma | \phi_l(t) \rangle$ with $\sigma = \pm 1/2$. The coordinate space is a box whose x-, y-sides are 30 fm and z-side is 50 fm, discretized in the square mesh of $\Delta x = \Delta y = \Delta z = 1.0$ fm.

3. Results

We simulate the $^{20}\text{O}+^{20}\text{O}$ collision with incident energy $E_{\text{int}} = 40$ MeV which is higher than the Coulomb barrier in this system. Initial distance between projectile and target is 12 fm with $b = 0$ fm. ^{20}O ($Z=8$, $N=12$) has superfluidity for neutrons. The average gap-energy $\bar{\Delta} \equiv \sum_{l>0} \Delta_l / \sum_{l>0} 1$ is 1.901 MeV. The number of canonical basis is 24(1.2 times that of TDHF).

Figure 1 shows the time evolution of neutron density distributions. After the touch ($t = 98.66$ fm/c: panel (b) in Fig.1), the density-distribution vibrates keeping the prolate shape. This shape of a new mean field corresponds to the shape of ^{40}S ($Z=16$, $N=24$) ground state in intrinsic frame. Figure 2 shows the time-evolution of neutron gap-energy for each canonical basis defined in Eq.(2). From the touching configuration, the gap energies are decreasing significantly. The decrease is similar to the results of old work[6]. We can see the vibration of gap energies related with nuclear density behavior.

We simulated the $^{20}\text{O}+^{20}\text{O}$ collision using time-dependent mean field theory including the effects of nuclear superfluidity, and showed the vibration of gap energies in the collision. Currently, we are investigating the detail of gap energy vibration and relation with the excited states of ^{40}S . To study the pairing effects for collision phenomena, we should improve our program code to parallel one. We parallelize the code using MPI for the canonical basis, because the canonical basis conserve orthogonality in the Cb-TDHF which means they do not need Gram-Schmidt orthonormalization in the real time-evolution. We can expect the parallelization efficiency of the method is good, due to the relatively small communication-loss.

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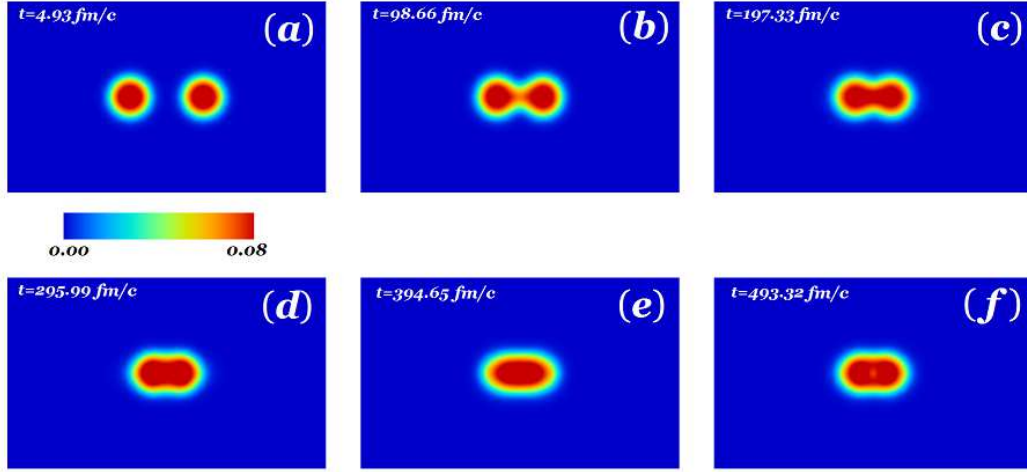


Figure 1. Neutron density distributions of XZ-plane in $^{20}\text{O}+^{20}\text{O}$ collision at $t=(a)4.93$, $(b)98.66$, $(c)197.33$, $(d)295.99$, $(e)394.65$ and $(f)493.32$ fm/c. The horizontal direction corresponds to Z direction.

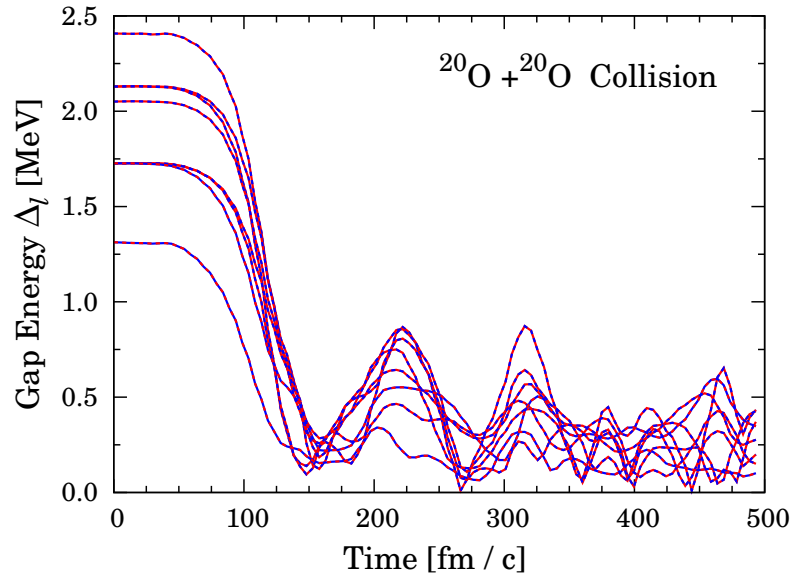


Figure 2. Time-evolution of neutron gap-energy defined in Eq.(2). Solid lines (red online) and dashed lines (blue online) indicate the gap energies of l -states in target and projectile nuclei, respectively.